Thermochemistry of Liquid Organic Hydrogen Carrier: How Calorimetry sets the foundations for development of the technology

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Liquid Organic Hydrogen Carrier (LOHC) are an attractive option for the storage of hydrogen. Hydrogen is stored by the reversible hydrogenation of an aromatic substance (the hydrogen-lean form), forming the corresponding saturated derivative (the hydrogen-rich form). The covalent bond enables storage at ambient conditions in a safe and dense form. Hydrogen release is done catalytically in an endothermal dehydrogenation reaction.

Several substances have been proposed as LOHC materials. For the selection of suited candidates, caloric properties are of utmost importance. In theory, all unsaturated components could be utilized. However, for reasonable conditions in the hydrogen release reactor, it is important to find substances with enthalpies of reaction of about +40 kJ mol$(H_2)^{-1}$ for the dehydrogenation. Yet, most materials have enthalpy values higher than this (often between +55 and +70 kJ mol$(H_2)^{-1}$).

Systematic search for suited carrier materials therefore requires consistent data sets regarding enthalpies of formation. Particularly data for the hydrogenated forms are often not available or the quality of the respective data is questionable. Hence, LOHC research is highly depending on an improved data base for caloric properties of potential LOHC candidates.

Experimental data still play a vital role in this regard and are crucial for obtaining reliable data. However, nowadays predictive methods, such as quantum-chemistry based approaches, are becoming increasingly more relevant. They do not only provide a shortcut method for obtaining data experimentally not available, but can also help to validate experimental data for LOHC materials and extend their range of applicability.